

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 04.11.2010

Version 3.5

### 1. Identification of the substance/mixture and of the company/undertaking

#### 1.1 Product identifier

Catalogue No.	820730
Product name	Iodobenzene for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

#### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merck-chemicals.com">www.merck-chemicals.com</a> ).
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#### 1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

**1.4 Emergency telephone number**      **Please contact the regional company representation in your country.**

### 2. Hazards identification

#### 2.1 Classification of the substance or mixture

**Classification (REGULATION (EC) No 1272/2008)**

Acute toxicity, Category 4, Oral, H302

For the full text of the H-Statements mentioned in this Section, see Section 16.

**Classification (67/548/EEC or 1999/45/EC)**

Xn; R22

For the full text of the R-phrases mentioned in this Section, see Section 16.

#### 2.2 Label elements

**Labelling (REGULATION (EC) No 1272/2008)**

*Hazard pictograms*



*Signal word*

Warning

*Hazard statements*

H302 Harmful if swallowed.

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**Reduced labelling (≤125 ml)**

*Hazard pictograms*



*Signal word*  
Warning

CAS-No. 591-50-4

**Labelling (67/548/EEC or 1999/45/EC)**

Symbol(s)	Xn	Harmful
R-phrase(s)	22	Harmful if swallowed.
EC-No.	209-719-6	

**2.3 Other hazards**

None known.

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**3. Composition/information on ingredients**

Formula	C <sub>6</sub> H <sub>5</sub> I (Hill)
CAS-No.	591-50-4
EC-No.	209-719-6
Molar mass	204,01 g/mol

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**4. First aid measures**

**4.1 Description of first aid measures**

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

**4.2 Most important symptoms and effects, both acute and delayed**

We have no description of any toxic symptoms.

**4.3 Indication of immediate medical attention and special treatment needed**

No information available.

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**5. Fire-fighting measures**

**5.1 Extinguishing media**

*Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

*Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

**5.2 Special hazards arising from the substance or mixture**

Combustible material, Vapours are heavier than air and may spread along floors.

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Forms explosive mixtures with air on intense heating.  
Development of hazardous combustion gases or vapours possible in the event of fire.  
Fire may cause evolution of:  
hydrogen iodide

### 5.3 Advice for firefighters

#### *Special protective equipment for fire-fighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

#### *Further information*

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## 6. Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Ensure adequate ventilation. Avoid substance contact. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

### 6.2 Environmental precautions

Do not empty into drains.

### 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7.2 and 10.5).

Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## 7. Handling and storage

### 7.1 Precautions for safe handling

Observe label precautions.

### 7.2 Conditions for safe storage, including any incompatibilities

Tightly closed. Protected from light.

Store at +15°C to +25°C.

### 7.3 Specific end uses

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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## 8. Exposure controls/personal protection

### 8.1 Control parameters

### 8.2 Exposure controls

Engineering measures

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Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

**Individual protection measures**

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

*Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

*Eye/face protection*

Safety glasses

*Hand protection*

full contact:

Glove material:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 10 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 890 Vitoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet (>,<) supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

*Respiratory protection*

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

*Environmental exposure controls*

Do not empty into drains.

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**9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

Form	liquid
Colour	yellow
Odour	No information available.

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Odour Threshold	No information available.
pH	No information available.
Melting point	-30 °C
Boiling point/boiling range	187 - 189 °C
Flash point	77 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	1,41 hPa at 25 °C (experimental)
Relative vapour density	No information available.
Relative density	1,83 g/cm <sup>3</sup> at 20 °C
Water solubility	0,34 g/l at 30 °C (experimental)
Partition coefficient: n-octanol/water	log Pow: 3,25 Method: (experimental) (Lit.) A remarkable bioaccumulation potential is expected (log Po/w >3).
Autoignition temperature	No information available.
Decomposition temperature	> 200 °C explosion decomposition
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Oxidizing properties	No information available.

## 9.2 Other data

none

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## 10. Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

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**10.2 Chemical stability**

Sensitivity to light

**10.3 Possibility of hazardous reactions**

Violent reactions possible with:

Strong oxidizing agents

**10.4 Conditions to avoid**

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

**10.5 Incompatible materials**

no information available

**10.6 Hazardous decomposition products**

in the event of fire: See chapter 5.

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**11. Toxicological information**

**11.1 Information on toxicological effects**

*Acute oral toxicity*

LD50 rat

Dose: 1.749 mg/kg

(RTECS)

Symptoms: We have no description of any toxic symptoms.

absorption

*Acute inhalation toxicity*

LC50 rat

Dose: 16,32 mg/l

(RTECS)

*Sensitisation*

Sensitization possible in predisposed persons.

*Specific target organ toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

*Specific target organ toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

*Aspiration hazard*

No aspiration toxicity classification

**11.2 Further information**

*Further information*

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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**12. Ecological information**

**12.1 Toxicity**

No information available.

**12.2 Persistence and degradability**

No information available.

**12.3 Bioaccumulative potential**

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*Partition coefficient: n-octanol/water*

log Pow: 3,25

Method: (experimental)

(Lit.) A remarkable bioaccumulation potential is expected (log Po/w >3).

#### 12.4 Mobility in soil

No information available.

#### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

#### 12.6 Other adverse effects

*Additional ecological information*

We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Do not allow to run into surface waters, wastewater, or soil.

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### 13. Disposal considerations

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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### 14. Transport information

Not classified as dangerous in the meaning of transport regulations.

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### 15. Regulatory information

#### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

*EU regulations*

Major Accident Hazard

96/82/EC

Legislation

Directive 96/82/EC does not apply

Occupational restrictions

Take note of Dir 94/33/EC on the protection of young people at work. Take note of Dir 92/85/EEC on the safety and health at work of pregnant workers.

*National legislation*

Storage class VCI

10 Combustible liquids not in Storage Class 3

#### 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

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### 16. Other information

**Full text of H-Statements referred to under sections 2 and 3.**

H302

Harmful if swallowed.

**Full text of R-phrases referred to under sections 2 and 3**

R22

Harmful if swallowed.

#### **Training advice**

Provide adequate information, instruction and training for operators.

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Regional representation: This information is given on the authorised Safety Data Sheet for your country.

**Key or legend to abbreviations and acronyms used in the safety data sheet**

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*